

Homology Modelling of Beta Defensin 3 of Bos taurus and Its Docking Studies with Molecules Responsible for Formation of Biofilm

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Abstract : The Bos taurus Beta defensin 3 is a defensin peptide secreted by neutrophils and epithelial that exhibits anti-microbial activity. It is one of the crucial components forming an innate defense against intra mammary infections in livestock. The beta defensin 3 by virtue of its anti-microbial activity inhibits major mastitis pathogens including Staphylococcus aureus and Pseudomonas aeruginosa etc, which are also responsible for biofilm formation leading to antibiotic resistance phenomenon. Therefore, the defensin may prove as a non-conventional option to treat mastitis. In this study, computational analysis has been performed including sequence comparison among species and homology modeling of Bos taurus beta defensin 3 protein. The assessments of protein structure were done using the protein structure and model assessment tools integrated in Swiss Model server, which employs various local and global quality evaluation parameters. Further, molecular docking was also carried out between the defensin peptide and the components of biofilm to gain insight into various interactions and structural differences crucial for functionality of this protein.

Keywords : beta defensin 3, bos taurus, docking, homology modeling

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